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Image Construction for Concave Gratings at Grazing Incidence, by Ray Tracing

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The images formed by a concave grating used at grazing incidence are constructed by a ray-tracing method. The method, equivalent to a recently developed procedure of Spencer and Murty, can be used for any configuration of grating and object. The results are compared with a third-order approximate theory for the case of rays parallel to the Rowland plane.

INTRODUCTION

RECENTLY, the imaging properties of diffraction gratings have been discussed from several points of view. Namioka[1,2] has studied the aberrations of concave gratings, using Fermat's principle. Spencer and Murty[3] have developed a general ray-tracing procedure which includes gratings as elements of complete optical systems.

In the present work a ray-tracing method equivalent to that of Spencer and Murty is used to obtain the images formed by a concave grating used at grazing incidence, a configuration which is very important in space spectroscopy.

The results are compared with computations using an equation derived by Behring[4] from Fermat's principle for the special case of light rays initially parallel to the Rowland plane.

LIST OF SYMBOLS

$A(X,Y,Z)$—object point
$B(x,y,z)$—image point
$P(x_1,y_1,z_1)$—point on grating
$C(R,0,0)$—center of curvature of grating
D—vector with direction cosines as components
$p=[z_1^2+(R-x_1)^2]^{-\frac{1}{2}}$
$q=[(R-x_1)^2+y_1^2+z_1^2]^{-\frac{1}{2}}$
$\mathbf{\Lambda}$=matrix of transformation between (x,y,z) and (x',y',z') systems
A=matrix of quadric coefficients

DESCRIPTION OF METHOD

From any specified object point (X,Y,Z) (which need not be on the Rowland cylinder) a ray is constructed which impinges on the grating at the point $(x_1y_1z_1)$. The elemental part of the grating centered on $(x_1y_1z_1)$ is considered to be a plane grating whose plane is that of the tangent plane to the spherical surface (Fig. 1); the rulings on this elemental plane grating are the projection of the actual rulings on to the tangent plane. The direction of the resulting diffracted ray is then determined by the diffraction equation[5]

$$m\lambda/\sigma=(\sin\alpha+\sin\beta)\cos\delta, \tag{1}$$

in which the parameters α,β,δ are computed relative to the elemental plane grating, as illustrated in Fig. 2.

The intersection of the diffracted ray with any desired surface is then obtained and is the image point corresponding to the given incident ray. This imaging surface is usually the Rowland cylinder, or a cylinder centered on the grating in the case of an exit slit whose plane is normal to the grating pole–slit line.

In this way, by having incident rays from one object point impinge on a net of points on the grating, and repeating this process for a desired net of object points, the image distribution is obtained.

DETAILS OF CALCULATION

Derivation of Elemental Grating

In the following, each point such as $A(X,Y,Z)$ is considered to have vector **A** associated with it, the components of **A** being (X,Y,Z).

Let the object point be $A(X,Y,Z)$: the incident ray from it to an arbitrary point $P(x_1y_1z_1)$ on the grating

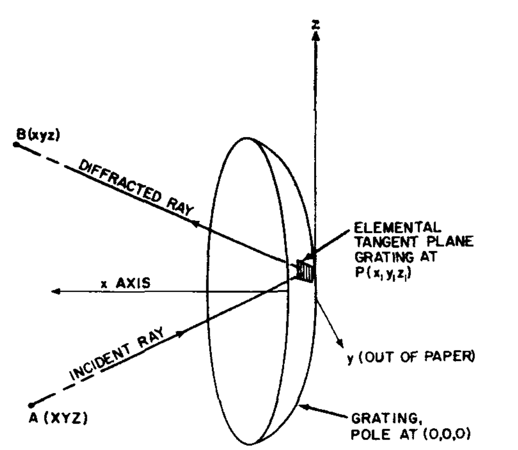

FIG. 1. Concave grating and coordinate system, illustrating also an elemental tangent plane grating.

[1] T. Namioka, J. Opt. Soc. Am. 49, 446 (1959).
[2] T. Namioka, J. Opt. Soc. Am. 49, 460 (1959).
[3] G. H. Spencer and M. V. R. K. Murty, J. Opt. Soc. Am. 52, 672 (1962).
[4] W. E. Behring (private communication).
[5] C. S. Rupert, J. Opt. Soc. Am. 42, 779 (1952).

has the parametric line equation

$$\mathbf{x}=\mathbf{P}+\frac{s(\mathbf{A}-\mathbf{P})}{[(X-x_1)^2+(Y-y_1)^2+(Z-z_1)^2]^{\frac{1}{2}}}, \qquad (2)$$

where s is the distance of point $\mathbf{x}(x,y,z)$ from P.

If $C(R,0,0)$ is the center of curvature of the grating, then the normal at P has the equation:

$$\mathbf{x}=\mathbf{P}+\frac{s(\mathbf{C}-\mathbf{P})}{[(R-x_1)^2+y_1^2+z_1^2]^{\frac{1}{2}}}, \qquad (3)$$

where s is the distance of point $\mathbf{x}(x,y,z)$ from P along the normal.

Since the grating sphere equation is

$$(x-R)^2+y^2+z^2=R^2, \qquad (4)$$

the equation of the tangent plane at $P(x_1y_1z_1)$ is

$$(x_1-R)(x-R)+y_1y+z_1z=R^2. \qquad (5)$$

The equation of the projection of the ruling at $P(x_1y_1z_1)$ onto this tangent plane results from the intersection of the plane $y=y_1$ with this tangent plane, being therefore

$$(x_1-R)(x-R)+y_1^2+z_1z=R^2. \qquad (6)$$

Application of Grating Equation

The tangent plane, with projected rulings on it, is the elemental plane diffraction grating mentioned earlier. The incident ray at $P(x_1y_1z_1)$ produces a diffracted ray leaving this elemental grating according to the equation

$$m\lambda/\sigma_e=(\sin\alpha+\sin\beta)\cos\delta, \qquad (7a)$$

where

$$\sigma_e=\sigma/[1-(y_1/R)^2]^{\frac{1}{2}}, \qquad (7b)$$

σ_e being a slowly varying function of y_1 because the actual ruling does not have a constant separation in the assumed type of grating. The reference plane in which α and β are measured is the plane through $P(x_1y_1z)$ which is normal to the line (6). This plane is now considered to be the x', y' plane of a new coordinate system $(x'\,y'\,z')$, whose x' axis is the grating normal at P, and whose z' axis is the projected line (6).

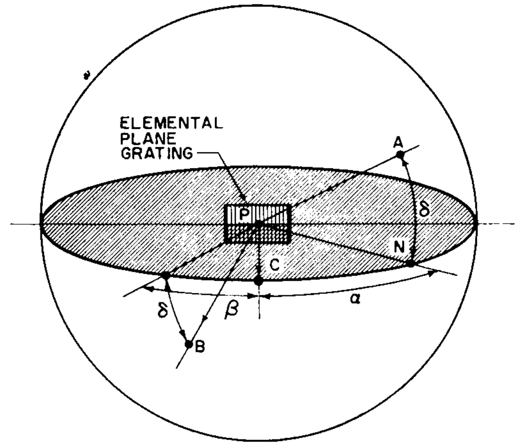

FIG. 2. Angles of diffraction equation (1), referred to an elemental plane grating.

Thus the new z' axis has the direction cosine vector

$$\mathbf{D}^{z'}=\frac{1}{[z_1^2+(R-x_1)^2]^{\frac{1}{2}}}\begin{vmatrix} z_1 \\ 0 \\ R-x_1 \end{vmatrix}\equiv p\begin{vmatrix} z_1 \\ 0 \\ R-x_1 \end{vmatrix}; \qquad (8)$$

the new x' axis has the direction cosine vector

$$\mathbf{D}^{x'}=\frac{1}{[(R-x_1)^2+y_1^2+z_1^2]^{\frac{1}{2}}}\begin{vmatrix} R-x_1 \\ -y_1 \\ -z_1 \end{vmatrix}\equiv q\begin{vmatrix} R-x_1 \\ -y_1 \\ -z_1 \end{vmatrix}. \qquad (9)$$

The direction cosine vector of the new y' axis is obtained as the cross product of those above:

$$\begin{aligned}\mathbf{D}^{y'}&=\mathbf{D}^{z'}\times\mathbf{D}^{x'}\\&=pq\{\mathbf{i}[y_1(R-x_1)]+\mathbf{j}[z_1^2+(R-x_1)^2]+\mathbf{k}[-y_1z_1]\}.\end{aligned} \qquad (10)$$

The equation of the $x'y'$ plane in the original coordinates, it should be mentioned, is found to be

$$z_1x+(R-x_1)z-z_1R=0. \qquad (11)$$

We now can find the angle α for the incident ray AP, defined as the angle between its projection on the $x'y'$ plane and the x' axis. This projected line is most easily obtained by finding the projection N of point A onto the $x'y'$ plane and then forming the equation of line PN. The equation is found to be:

$$\mathbf{x}'=\mathbf{P}+\frac{s}{\{(X-Uz_1-x_1)^2+(Y-y_1)^2+[Z-U(R-x_1)-z_1]^2\}^{\frac{1}{2}}}\begin{vmatrix} X-Uz_1-x_1 \\ Y-y_1 \\ Z-U(R-x_1)-z_1 \end{vmatrix}, \qquad (12)$$

in which

$$U=\frac{z_1X+(R-x_1)Z-z_1R}{z_1^2+(R-x_1)^2}. \qquad (13)$$

The angle α of the diffraction formula (7a) is the angle between this line (12) and the normal (x' axis):

$$\cos\alpha=Vq\{[X-Uz_1-x_1][R-x_1]+[Y-y_1][-y_1]+[Z-U(R-x_1)-z_1][-z_1]\}, \qquad (14a)$$

in which

$$V=\{[X-Uz_1-x_1]^2+[Y-y_1]^2+[Z-U(R-x_1)-z_1]^2\}^{-\frac{1}{2}}. \quad (14b)$$

Similarly, the angle δ of the diffraction formula is the angle between PA and PN and is therefore given by

$$\cos\delta=VW\{[X-Uz_1-x_1][X-x_1]+[Y-y_1]^2+[Z-U(R-x_1)-z_1][Z-z_1]\}, \quad (15a)$$

in which

$$W=[(X-x_1)^2+(Y-y_1)^2+(Z-z_1)^2]^{-\frac{1}{2}}. \quad (15b)$$

The diffraction angle β, in the new coordinate system $(x'y'z')$, can now be obtained as

$$\sin\beta=(m\lambda/\sigma_e\cos\delta)-\sin\alpha. \quad (16)$$

To get the direction of the diffracted ray in the $(x'y'z')$ system, then, we must rotate some point initially on the x' axis through an angle β in the PCN plane, and then perform a second rotation on the point to bring it out of the plane by the angle δ, both rotations being performed in appropriate directions. The situation is illustrated in Fig. 2. This is the usual transformation in spherical polar coordinates (r,θ,ϕ):

$$\begin{aligned} x&=r\sin\theta\cos\phi,\\ y&=r\sin\theta\sin\phi,\\ z&=r\cos\theta, \end{aligned} \quad (17)$$

except that here $\delta=(\pi/2)-\theta$, $\beta=\phi$, so that

$$\begin{aligned} x'&=\cos\delta\cos\beta,\\ y'&=\cos\delta\sin\beta,\\ z'&=\sin\delta, \end{aligned} \quad (18)$$

taking (1,0,0) as the original point on the x' axis. It should be noted that the sign of δ must always be taken opposite to that of the z' coordinate of the object point A.

Now, (x',y',z') are the coordinates of a point x_D' on the diffracted ray, in the new system. To obtain this point's coordinates in the original system we must transform these coordinates by the matrix

$$\mathbf{\Lambda}=\begin{vmatrix} D_x^{x'} & D_x^{y'} & D_x^{z'}\\ D_y^{x'} & D_y^{y'} & D_y^{z'}\\ D_z^{x'} & D_z^{y'} & D_z^{z'} \end{vmatrix}. \quad (19)$$

Thus, the coordinates of this point in the (x,y,z) system are

$$\mathbf{x}_D=\begin{vmatrix} D_x^{x'}\cos\delta\cos\beta+D_x^{y'}\cos\delta\sin\beta+D_x^{z'}\sin\delta\\ D_y^{x'}\cos\delta\cos\beta+D_y^{y'}\cos\delta\sin\beta+D_y^{z'}\sin\delta\\ D_z^{x'}\cos\delta\cos\beta+D_z^{y'}\cos\delta\sin\beta+D_z^{z'}\sin\delta \end{vmatrix}+\begin{vmatrix} x_1\\ y_1\\ z_1\end{vmatrix}, \quad (20)$$

remembering that the origin of the (x',y',z') system is the point $P(x_1y_1z_1)$.

The equation of the diffracted ray is now written down as

$$\mathbf{x}=\mathbf{P}+s(\mathbf{x}_D-\mathbf{P})T, \quad (21)$$

where T is a normalizing factor.

IMAGE POINTS

To find the intersection of this diffracted ray with the Rowland cylinder, we can conveniently use the matrix method described by Heading[6] as follows. If the line equation is $\mathbf{w}=\mathbf{w}_1+s\mathbf{h}$, and the quadric equation is $\mathbf{w}^{\mathrm{T}}A\mathbf{w}=0$, where $\mathbf{w}_1$ does not lie on the quadric, then the intersection values of s are given by

$$(\mathbf{w}_1^{\mathrm{T}}+s\mathbf{h}^{\mathrm{T}})A(\mathbf{w}_1+s\mathbf{h})=0 \quad (21a)$$

or, expanding,

$$\mathbf{w}_1^{\mathrm{T}}A\mathbf{w}_1+s(\mathbf{h}^{\mathrm{T}}A\mathbf{w}_1+\mathbf{w}_1^{\mathrm{T}}A\mathbf{h})+s^2\mathbf{h}^{\mathrm{T}}A\mathbf{h}=0 \quad (21b)$$

In the notation of the present problem, this equation is:

$$\mathbf{P}^{\mathrm{T}}A\mathbf{P}+2s\mathbf{L}^{\mathrm{T}}A\mathbf{P}+s^2\mathbf{L}^{\mathrm{T}}A\mathbf{L}=0, \quad (22)$$

where:

$$\mathbf{P}=\begin{vmatrix} x_1\\ y_1\\ z_1\\ 1\end{vmatrix}, \quad (23)$$

A for the Rowland cylinder is

$$A=\begin{vmatrix} 1 & 0 & 0 & -R/2\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 0\\ -R/2 & 0 & 0 & 0 \end{vmatrix}, \quad (24)$$

and the components of $\mathbf{L}$ are

$$\begin{aligned} \mathbf{L}_x&=T[q(R-x_1)\cos\delta\cos\beta+pqy_1(R-x_1)\cos\delta\sin\beta+pz_1\sin\delta] &&\equiv TH,\\ \mathbf{L}_y&=T\{q(-y_1)\cos\delta\cos\beta+pq[z_1^2+(R-x_1)^2]\cos\delta\sin\beta\} &&\equiv TJ,\\ \mathbf{L}_z&=T[q(-z_1)\cos\delta\cos\beta+pq(-y_1z_1)\cos\delta\sin\beta+p(R-x_1)\sin\delta] &&\equiv TK, \end{aligned} \quad (25a)$$

in which

$$T=(H^2+J^2+K^2)^{-\frac{1}{2}}. \quad (25b)$$

If the intersection of the diffracted ray with a grating-centered cylinder of radius r is desired, A is given instead by

[6] J. Heading, *Matrix Theory for Physicists* (Longmans Green and Company, Inc., New York, 1958), Chap. III.

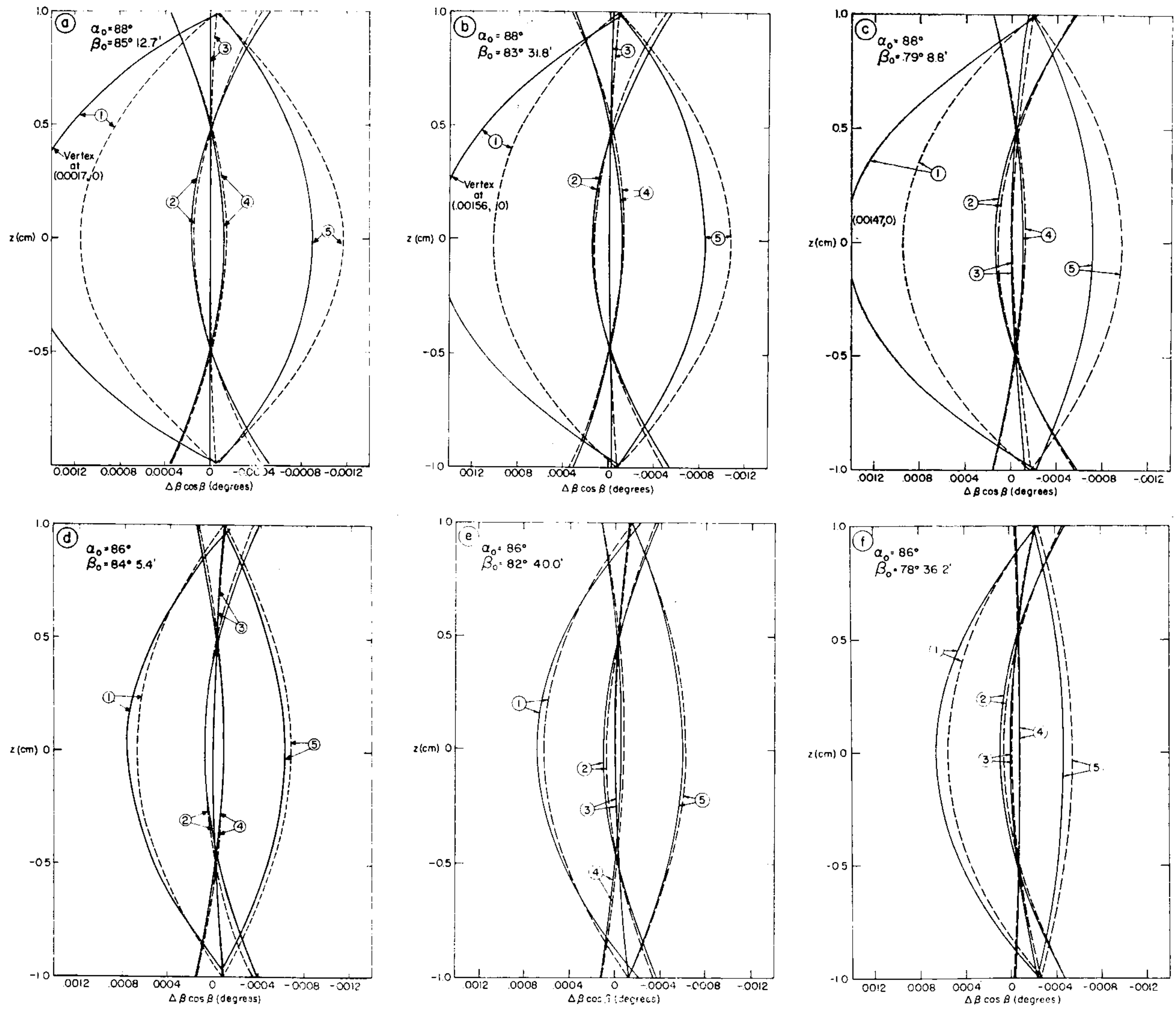

FIG. 3. Images (solid line) obtained by ray-tracing method compared with images (dashed line) obtained from third-order theory (diffraction order $m=+1$). Curves are illustrated for values of y_1/R of: (1) -0.01, (2) -0.005, (3) 0.0, (4) 0.005, (5) 0.01.

$$A=\begin{vmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & -r^2\end{vmatrix}. \tag{26}$$

The algebraically larger value of s is used in all cases.

COMPUTER USE OF THE EQUATIONS

For a given angle of incidence, a single central ray is calculated; i.e., the incident ray lying in the Rowland plane and impinging on the pole (0,0,0) of the grating. The intersection of the diffracted ray with the Rowland cylinder is found. This gives the radius r_c of the grating-centered cylinder upon which the image is to be formed, assuming that we want the image in a surface normal to the line from the image to the grating pole. A multiple run can then be made using a net of i object points, and a net of j grating points for each object point. Thus $i\cdot j$ image points are obtained.

APPLICATION TO A SPECTROMETER

The procedure developed in the foregoing sections has been applied to the problem of image formation in a grazing incidence spectrometer designed for observation of the solar extreme ultraviolet spectrum from the first orbiting solar observatory. This case corresponds to observation of an extended source at a very great distance from the entrance slit. Under such circumstances a beam of nearly parallel radiation from each element of the source illuminates the entire entrance slit so that the direction cosines for the incident rays from a specified element of the source can be taken as the same for every point on the grating which is illuminated

TABLE I. Values of β_0, the central ray diffraction angles, corresponding to angles of incidence α_0 and wavelength λ used for the curves of Fig. 3 ($m=+1$).

α_0 \ λ	50 Å	100 Å	300 Å
88°	85° 12.7	83° 31.8	79° 8.8
86°	85° 5.4	82° 40.0	78° 36.2

through the (infinitely narrow) entrance slit. For ease of comparison with an approximate (third-order) theory, it is assumed that the beam of radiation is parallel to the Rowland plane. This is justified only because in the case being considered (observation of the sun), the maximum deviation from this plane is only 0.005 rad.

Rays satisfying the above assumptions were selected from a more general machine ray tracing computation for angles of incidence of 88° and 86°. The results are given in Fig. 3 for several different values of the angle of diffraction β_0. In each case a 5×5 net of grating points was used corresponding to values of $y_1/R=0$, ±0.005, ±0.01, where y_1 is the horizontal distance of the illuminated grating point from the pole of the grating and R is the radius of curvature of the grating. The distances of the grating points from the Rowland plane were taken as 0, ±0.5, and ±1.0 cm. For $\sigma=0.00017361$ cm, $R=100$ cm the wavelengths corresponding to values of β_0 specified in Fig. 3 are given in Table I. Values of $\Delta\beta\cos\beta$ are directly convertible into $\Delta\lambda$ using the differentiated grating equation. The values of $y_1/R=\pm0.005$ correspond to images formed by those portions of the solar limb lying in the Rowland plane and represent the maximum deviations from the image formed by the central ray from the center of the sun.

It should be pointed out that these images are obtained for the specified values of α and β in any grating system for values of y_1/R equal to 0.01 and 0.005. The values of wavelength for which the results apply are found using the grating equation.

An inspection of the figures reveals the improvement in image quality obtained either by reducing the angle of incidence α or the value y_1/R. They show also how the curves based on third-order theory depart from the exact ray-traced results as the angle of incidence increases.

CONCLUSIONS

The ray-tracing method developed for a concave grating enables one to obtain image shapes for all configurations in which a concave grating may be used; it can be used equally well at near normal incidence or at grazing incidence. It serves therefore as a standard of comparison against which approximate theories can be tested.

Because of the "closed" nature of the calculation, making its use in a computer program convenient, it is possible to generate quickly as many images as may be required for spectrometer design purposes. A few such images have been presented above for the OSO extreme ultraviolet spectrometer.

ACKNOWLEDGMENTS

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